3,4-Dihydroxyacetophenone
1197-09-7 | DTXSID30152546

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 255 °C

Global applicability domain: Inside

Local applicability domain index: 4.18e-01

Confidence level: 7.56e-01

Nearest Neighbors from the Training Set

Image not found

2,3-Dihydroxybenzaldehyde
Measured: 235
Predicted: 253

Image not found

4-Isopropylcatechol
Measured: 271
Predicted: 277

Image not found

1,2-Benzenediol, 3-methyl-
Measured: 241
Predicted: 257

Image not found

4-Methylcatechol
Measured: 251
Predicted: 257

Image not found

4-tert-Butylcatechol
Measured: 285
Predicted: 277